

2-Benzyl-2,3-dihydro-1H-pyrrolo[3,4-c]pyridine
368441-96-7 | DTXSID50364048

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 8.09

Global applicability domain: Inside

Local applicability domain index: 4.88e-01

Confidence level: 5.81e-01

Nearest Neighbors from the Training Set

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4-Isobutylmorpholine

Measured: 1.78

Predicted: 2.69

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Molinate

Measured: 25.7

Predicted: 14.8

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N,N-Dimethyl-1,2-dithiolan-4-amine

Measured: 52.5

Predicted: 17.5

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Triethylamine

Measured: 4.90

Predicted: 5.95

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2,2-Bis(bromomethyl)-1,3-propanediol

Measured: 4.79

Predicted: 3.35